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Artificial intelligence-assisted design of new chemical materials: a perspective

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New chemical materials are a fresh category of substances created through chemical reactions or by refining existing materials through secondary processes. By using creative methods, advanced technologies, innovative techniques, and state-of-the-art equipment, these materials (e.g., high-end polyolefin, nano materials) [1] are carefully designed and developed to showcase outstanding performance and unique capabilities beyond what traditional chemical materials can offer [2]. They possess characteristics such as light weight, impressive functionalities, strong performance, and high technological value. These materials serve as the building blocks of advanced foundational materials, hold significant strategic importance, and represent the forefront of cutting-edge innovations in materials science. Nevertheless, the progress in researching and developing new chemical materials frequently falls behind, resulting in a delay in meeting the demands of various applications [3]. It is crucial to establish a novel design paradigm for new chemical materials and even other fields that can bring about a transformation in the methods of researching and producing new materials for practical usage [4, 5].

Up to now, materials science research has undergone four paradigms: empirical, theoretical, computational, and data-driven, as illustrated in Figure 1(a) [6]. The first paradigm (empirical science) relies on trial-and-error experiments drawing from researchers' accumulated experience, while suffering from low efficiency and resource-intensive processes. The second paradigm (theoretical science) involves creating scientific laws and theories based on past experiences, providing a theoretical basis to improve trial-and-error methods, however, it may oversimplify complex material systems. The third paradigm (computational science) uses computer simulations of atomic or molecular interactions, to understand macroscopic properties, but requires significant computational resources. The fourth paradigm (data-driven science) entails intelligent analysis of extensive data using algorithms to reveal hidden connections between data points. At present, the primary method for developing new chemical materials continues to be empirical or theoretical trial-and-error approaches, demanding ongoing experimentation and repetitive trials to navigate vast chemical structures [3].

In sharp contrast, the fourth paradigm, anchored in data-driven methods and synergized with the earlier three paradigms, revolves prominently around the fusion of theoretical calculations, database technologies, and, most notably, artificial intelligence (AI), all in tandem with traditional experiments. AI empowers the analysis of the vast data, uncovering complex patterns and relationships that might elude human perception alone, and it has been widely applied in various fields (e.g., autonomous vehicles, industrial manufacturing) [7–9]. The ultimate objective of applying AI is twofold: to expedite the pace of new material discovery and to significantly trim the expenditures entailed in research endeavors. By enabling AI in the entire life cycle of new chemical material design, the transformation of the research and development paradigm for new materials is achieved through optimal structural design for product performance; the functionality and performance of new material products are enhanced through building a regulatory mechanism for consistent product quality and the maximization of the high-end value chain in the industrial ecosystem is ensured through developing comprehensive quality-benefit optimization decision solutions [10]. AI-assisted design propels the metamorphosis of new chemical materials, realizing intelligent digitization in design, elevating it to a high-end and high-value paradigm, and achieving green and low-carbon transformation. This endeavor inherently aligns with the concepts of digital transformation, the digital economy, and the industrial metaverse [11].

In addition, human knowledge and other social elements are now integral throughout the entire life cycle of the AI-assisted design for new chemical materials [12]. These factors have become crucial and can even play a decisive role at every stage of real-world process industries. The interactions between cyber-physical-social system (CPSS) and these societal factors are illustrated in Figure 1(a), and we also demonstrate a simple development cycle for new chemical materials with AI in CPSS.

CPSSs [13–15] will carry out parallel execution and self-synchronization, and influence the physical, information, cognitive, and social domains. Technically, CPSSs can excavate the inner principles of technology from the micro level and form the overall structure of designing new chemical materials from the macro level. Leveraging human knowledge [16] across design, production, and man-

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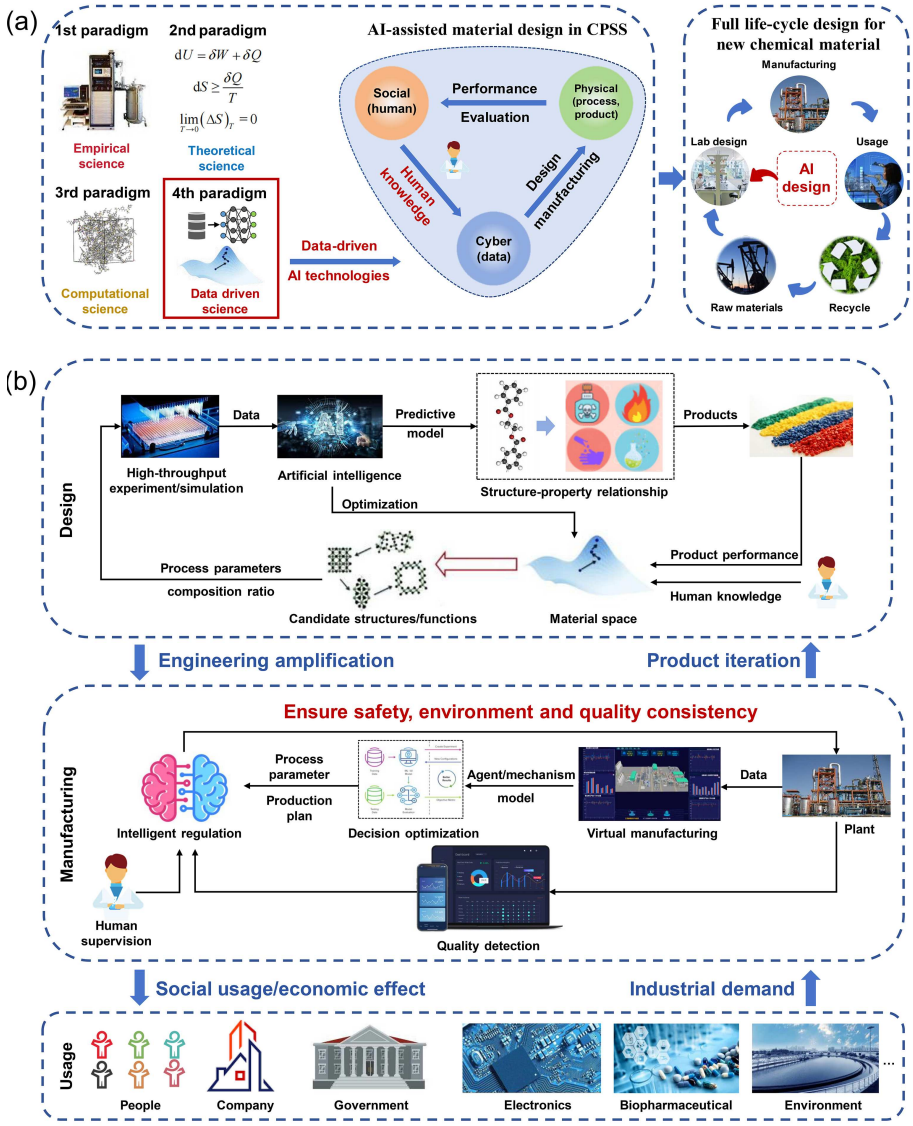

Figure 1 (Color online) (a) Four paradigms for material design and overview of AI-assisted material design with cyber-physical-social system (left). To accelerate the process of developing new chemical materials, it is urgent to apply AI-based technology in data-driven science to realize intelligent design in the entire cycle of material design. Here, we show a simple demonstration for new chemical material with an AI-assisted design framework (right). (b) Main process of designing new chemical materials, including the phases of design, manufacturing, and usage. Human knowledge is fully utilized to accelerate the entire process.

agement, alongside knowledge-based automation technology, holds the promise of driving smart manufacturing and informed decision-making.

In this study, we design an entire circle for designing new chemical materials in CPSS, shown in Figure 1(b), including the phase of design, manufacture, and usage. For design, high-throughout techniques provide a large amount of cyber data to learn potential structure-activity relationships assisted with AI techniques, e.g., machine learning, deep learning, and reinforcement learning. Then, all sub-optimal candidates are filtered out for physical production, and according to product performance and human guidance, the model is further optimized to search for better process parameters when engineering amplification. For manufacturing, human supervision is integrated with quality cyber characterization and detection to ensure safety, stability, and quality consistency for physical devices to adjust corresponding process parameters. For usage, with production iteration, new products will generate positive economic effects and boost the development of various fields, including electronics, medical, and the environment. To understand the thought patterns related to the proposed CPSS framework for designing new chemical materials, we conclude the following challenging research topics for the near future.

(1) Visualization and digitization: Designing cutting-edge simulations enables precise 3D modeling of molecular structures, allowing researchers to visualize intricate details. Applying virtual reality and metaverse technologies offers immersive experiences, aiding in the comprehension of complex molecular arrangements in materials. Efficient visualization and digitization-driven approach facilitate tailored materials design with enhanced accuracy and efficiency, forming a core pillar of the multidisciplinary process.

(2) Industrial intelligence: To build reliable industrial in-

telligence, sophisticated AI-based algorithms, multi-source data acquisition mechanism, few-shot learning, domain-specific large models fine-tuned by existing models or trained from scratch (e.g., polyBERT [16], ChatGPT [17]) should be developed for accurate property predictions and dynamic processes optimization. Assurance mechanisms should also be considered for real-time adjustments to ensure reliability and safety. This intelligent integration of information and physical processes enhances efficiency and innovation.

(3) Privacy protection: The concern for data privacy is quite common in the age of AI; thus blockchain and federated learning technologies can be further considered to create secure, decentralized data sharing mechanisms for collaborative research. This ensures that researchers collectively harness the power of data without compromising sensitive information, fostering trust and cooperation.

(4) Industrial software: To enhance the universality of the technology, integrated industrial software should be developed, realizing the functions discussed above. In addition, the journey from small-scale platforms or software to pilot testing and eventually scaling up to an enterprise level is a critical application transformation process to be considered.

In this study, a vision for designing new chemical materials towards a CPSS future is presented by fully incorporating human intelligence into existing traditional cyber and physical manufacturing systems. In the pursuit of future AI-assisted new chemical material design under full life circle, metaverse takes on a significant role. Imagine a collaborative virtual environment where researchers, engineers, and AI agents coexist seamlessly. This digital realm allows for real-time interactions, data sharing, and joint exploration of novel structures of new materials. Furthermore, blockchain technologies should be considered to protect the data privacy for fair distribution of credit and resources among collaborators. In addition, the visualization of material design is essential, and this capability enhances interdisciplinary communication and accelerates the convergence of diverse perspectives toward optimal material outcomes. To realize industrial intelligence, industrial large-scale models and multi-modal intelligence should be further researched, in the form of industrial software in the final. We hope that this perspective will help shape the thinking of the next generation of AI-assisted design pattern for new chemical materials.

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References

1 Kumar S, Wang Z, Zhang W, et al. Optically active nanomaterials and its biosensing applications—a review. Biosensors, 2023, 13: 85
2 Zheng Z P, Huang Y J, Wu F, et al. Multidimensional modulation of light fields via a combination of two-dimensional materials and meta-structures. Sci China Inf Sci, 2023, 66: 160403
3 Cheetham A K, Seshadri R, Wudl F. Chemical synthesis and materials discovery. Nat Synth, 2022, 1: 514–520
4 Law K L, Narayan R. Reducing environmental plastic pollution by designing polymer materials for managed end-of-life. Nat Rev Mater, 2022, 7: 104–116
5 Wang C, Liang J, Kim J T, et al. Prospects of halide-based all-solid-state batteries: From material design to practical application. Sci Adv, 2022, 8: eadc9516
6 Agrawal A, Choudhary A. Perspective: materials informatics and big data: Realization of the "fourth paradigm" of science in materials science. APL Mater, 2016, 4: 053208
7 Zhu G X, Lyu Z H, Jiao X, et al. Pushing AI to wireless network edge: an overview on integrated sensing, communication, and computation towards 6G. Sci China Inf Sci, 2023, 66: 130301
8 Zhang B, Zhu J, Su H. Toward the third generation artificial intelligence. Sci China Inf Sci, 2023, 66: 121101
9 Zhang Y, Carballo A, Yang H, et al. Perception and sensing for autonomous vehicles under adverse weather conditions: a survey. ISPRS J Photogrammetry Remote Sens, 2023, 196: 146–177
10 Wang H, Fu T, Du Y, et al. Scientific discovery in the age of artificial intelligence. Nature, 2023, 620: 47–60
11 Qian F. The future of smart process manufacturing. Engineering, 2023, 22: 20–22
12 Qian F, Tang Y, Yu X. The future of process industry: a cyber-physical-social system perspective. IEEE Trans Cybern, 2024, 54: 3878–3889
13 Liu L, Zhao X D, Wang B H, et al. Event-triggered state estimation for cyber-physical systems with partially observed injection attacks. Sci China Inf Sci, 2023, 66: 169202
14 Sun Q, Chen J C, Shi Y. Event-triggered robust MPC of nonlinear cyber-physical systems against DoS attacks. Sci China Inf Sci, 2022, 65: 110202
15 Wang X, Cheng X, Lu J, et al. Metaverses-based parallel oil fields in CPSS: a framework and methodology. IEEE Trans Syst Man Cybern Syst, 2023, 53: 2138–2147
16 Kuenneth C, Ramprasad R. polyBERT: a chemical language model to enable fully machine-driven ultrafast polymer informatics. Nat Commun, 2023, 14: 4099
17 Fu N, Wei L, Song Y, et al. Material transformers: deep learning language models for generative materials design. Mach Learn-Sci Technol, 2023, 4: 015001